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Uranium Density, Thermal Conductivity, Specific Heat, and Thermal Diffusivity

Seth D. Imhoff

22 February, 2021

This document is written using RMarkdown (Allaire et al. 2018; R Core Team 2018), meaning that all calculations are highly reproducible and available as relatively easy to read source code that includes text and analysis.

Introduction

Thermophysical properties for pure uranium are collected here as a common and maintained resource with a focus on casting.¹ Source material details will be provided for decisions on fitting emphasis. The four material properties represented in this document were chosen based upon the definition of thermal diffusivity (Eq. 1.1).²

$$\alpha \equiv \frac{k}{\rho \cdot c_p} \quad (\text{Eq. 1.1})$$

¹ The casting focus applies a natural influence on assumptions and ranges of validity

² Since each of the underlying parameters, including thermal diffusivity, can be measured independently it provides an important experimental check on each data set.

Symbols, Transitions, and Applicability

Use of symbols for material properties is inconsistent at best and downright confusing at worst. For the purposes of this document, one set of symbols will be used and all values provided in SI units.

Parameter	Symbol	SI Base	SI Equivalent
Temperature	T	K	
Thermal Diffusivity	α	$m^2 \cdot s^{-1}$	
Thermal Conductivity	k	$m \cdot kg \cdot s^{-3} \cdot K^{-1}$	$W \cdot m^{-1} \cdot K^{-1}$
Density	ρ	$kg \cdot m^{-3}$	
Specific Heat	c_p	$m^2 \cdot s^{-2} \cdot K^{-1}$	$J \cdot kg^{-1} \cdot K^{-1}$

Table 1: Symbols and units used in this document

The limits of applicability for the values reported here are confined to the equilibrium phase boundaries given in the table below at atmospheric pressure. Modest extrapolation of weakly varying or highly linear trends into metastable regimes is generally acceptable, but the accuracy is unknown.

Transition	Temperature	Enthalpy	Heat of...
α to β	942.02	6.641628×10^5	Transformation
β to γ	1048.99	1.1322136×10^6	Transformation
γ to Liquid	1407.99	2.1757793×10^6	Fusion
Liquid to Gas	4432.08	1.1836044×10^8	Vaporization

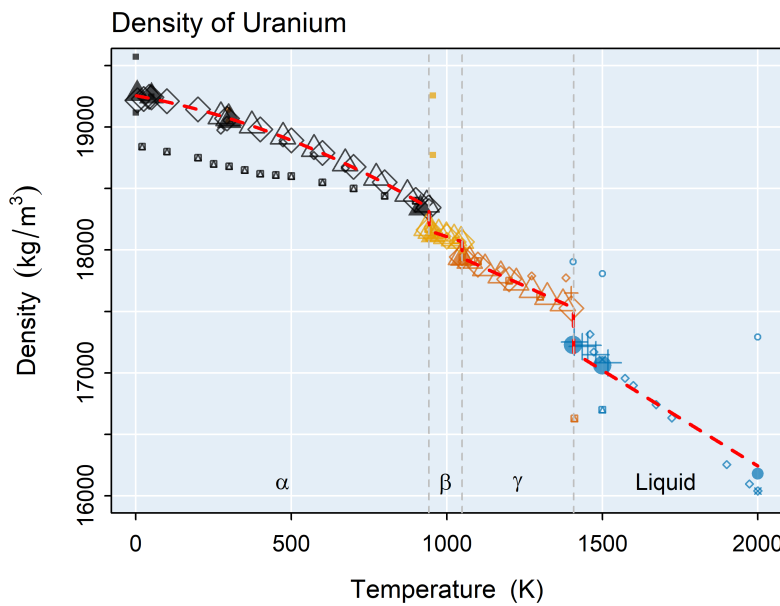
Table 2: Ideal phase transition temperatures as used within this document. Temperatures, Dinsdale (1991), reported in K and enthalpy, Turchi (2018), in J/kg.

Density

Density tends to monotonically decrease with increasing temperature with discontinuities at phase transitions. Experimentally, the presence of voids or second phase particles will alter the measured density as compared to the pure material. Due to the high atomic mass of uranium, mixed phases due to purity will nearly always decrease the apparent density of a sample. If high quality measurements of void volume fraction and second phase particle volume fraction are made, corrections to a measured density are appropriate.

Density is highly crystal structure dependent, therefore temperature regions are chosen based upon the allotropic phase transition temperatures given. The data may be fit to the following equation.

$$\rho(T) [kg \cdot m^{-3}] = A_0 + A_1T + A_2T^2 \quad (\text{Eq. 1.2})$$



Data and weighting updated 22 February, 2021

Figure 1: The density of depleted uranium as a function of temperature. Relative point sizes correspond to weight value for fitting, colors correspond to different phase regimes (Table 2) and shapes correspond to different sources. The red dashed line corresponds to the model described by Table 3.

Temperature (K)	A_0	A_1	A_2
$T > 1407.99$	1.9358119×10^4	-1.5574577	
$1048.99 < T \leq 1407.99$	1.9123305×10^4	-1.1326445	
$942.02 < T \leq 1048.99$	1.894995×10^4	-0.8413968	
$942.02 \leq T$	1.9254898×10^4	-0.4527681	$-5.4633007 \times 10^{-4}$

Table 3: Density temperature ranges and equation coefficients. Temperature in Kelvin and output is in $kg \cdot m^{-3}$.

Thermal Conductivity

The thermal conductivity of materials is controlled by phonon, electron, and electromagnetic interactions. Metals have a strong electronic component and so general trends between electrical conductivity (σ) and thermal conductivity are well defined by the Weidman-Franz law ($k/\sigma = LT$) where L is a constant known as the Lorenz number (Erez and Even (1966)).³

Behavior at cryogenic temperatures is highly non-linear. Pure metals will tend rise to a peak in the first 10s of degrees before becoming more linear. Purity and processing history can dominate measurements at low temperatures. For uranium, Hin (2018) points out the divergent trends in measurements at low temperatures which can also be observed in the plot given here. Model reliability fails below 43 K and should be considered suspect below the divergence of multiple measurements below 225 K.

³ Free electron theoretical value $L = 2.44 \times 10^{-8} \text{W}\Omega\text{K}^{-2}$ and at least one measurement reports $L \approx 3.0 \times 10^{-8} \text{W}\Omega\text{K}^{-2}$ at high temperature.

$$k[\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}] = K_0 + K_1T + K_2T^2 + K_3T^{-1} \quad (\text{Eq. 1.3})$$

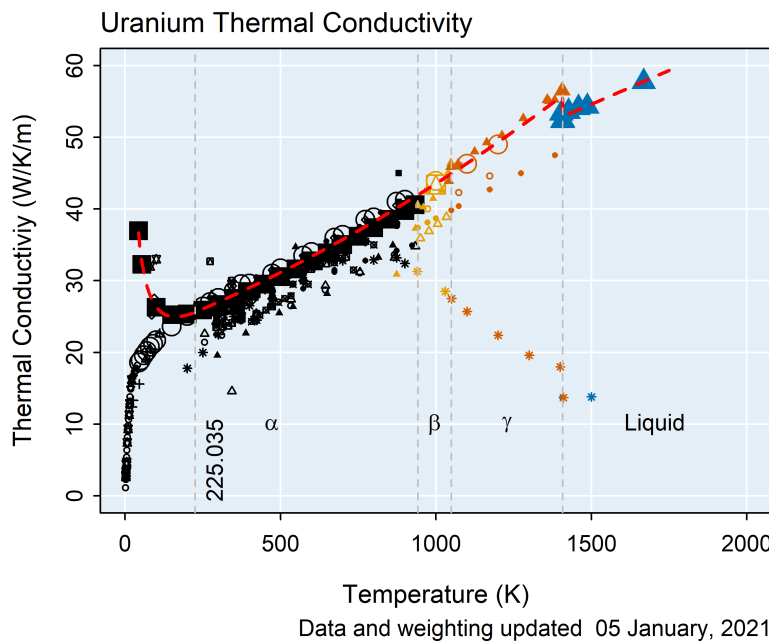


Figure 2: Thermal conductivity of uranium. Relative point sizes correspond to weight value for fitting, colors correspond to different phase regimes (Table 2) and shapes correspond to different sources. The red dashed line corresponds to the model described by Table 4.

Temperature (K)	K_0	K_1	K_2	K_3
$T > 1407.99$	26.3205746	0.0188604		
$225.035 < T \leq 1407.99$	21.73	1.591e-2	5.907e-6	
$225.035 \leq T$	10.3608201	0.0576244		596.8691497

Table 4: Thermal conductivity equation coefficients. Temperature is given in K and output is in W/K/m.

Specific Heat Capacity

Specific heat capacity is the amount of energy required to raise one kilogram of material by one degree and constitutes perhaps the most fundamental thermodynamic property because enthalpy and entropy are calculated from it. Increasing from zero, specific heat increases rapidly before increasing more modestly above the Debye temperature. At very low temperatures quantum effects can lead to highly non-linear behavior. At high temperatures, the smoothly increasing trend is punctuated by discontinuities at first order phase transitions as well as other higher order features.

In general, a bayesian information criterion is used to prevent overfitting. Specifically, the bic function from the stats package of R (R Core Team (2020)).]. The BCC phase was forced to a single value only because the ranges of the most reliable data were such that a slope would have resulted even though the investigators did not observe any temperature dependence.

$$c_p[J \cdot kg^{-1} \cdot K^{-1}] = C_{p,0} + C_{p,1}T + C_{p,2}T^2 + C_{p,3}T^3 + C_{p,4}T^{-2} \quad (\text{Eq. 1.4})$$

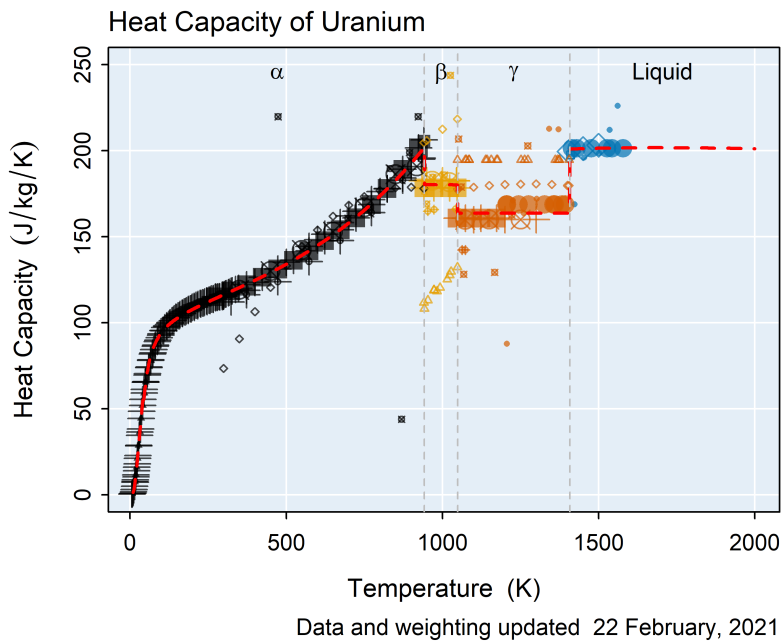


Figure 3: Specific heat capacity of uranium. Relative point sizes correspond to weight value for fitting, colors correspond to different phase regimes (Table 2) and shapes correspond to different sources. The red dashed line corresponds to the model described by Table 5.

	$T > 1407.99$	$1048.99 < T \leq 1407.99$	$942.02 < T \leq 1048.99$
$C_{p,0}$	258.8059861	163.6091401	181.7536164
$C_{p,1}$	-0.0396307	0	-0.0015739
$C_{p,2}$	9.0226665×10^{-6}	0	0
$C_{p,3}$	$-6.9036998 \times 10^{-10}$	0	0
$C_{p,4}$	-3.5921506×10^7	0	0

Table 5: Specific heat capacity equation coefficients listed for each temperature range following the form of the equation above. Temperature in Kelvin and output is in $J/kg/m^3$. This table is divided into two sections due to size.

	$43 < T \leq 942.02$	$T < 43$
$C_{p,0}$	94.7530785	5.0028476
$C_{p,1}$	0.0823891	-1.4155257
$C_{p,2}$	$-5.1158949 \times 10^{-5}$	0.1191441
$C_{p,3}$	8.9685518×10^{-8}	-0.0013435
$C_{p,4}$	-8.4542518×10^4	0

Thermal Diffusivity

Currently, the thermal diffusivity presented here is calculated by correlation (Eq. 1.1). Source data is used as a check on overall accuracy and to highlight areas in need of further investigation. Due to the uncertainty in the thermal conductivity, model outputs below 225 K should be used with caution and likely fail below 43 K.

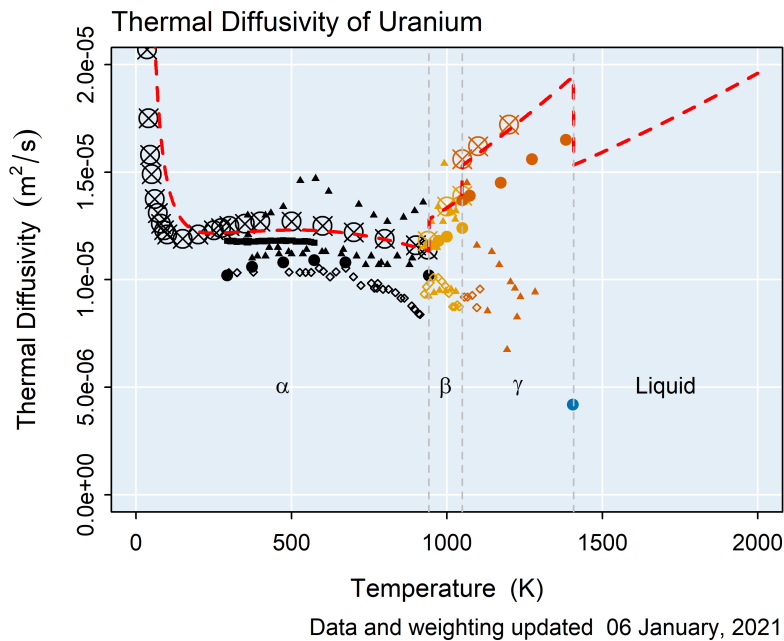


Figure 4: The thermal diffusivity of uranium as a function of temperature. Relative point sizes correspond to weight value for fitting, colors correspond to different phase regimes, Table 2, and shapes correspond to different sources. The red dashed line corresponds to the model described by Eq. 1.1 in concert with tables 3, 4 and 5.

Tabular Values of Properties

Temperature		Phase	Density
(K)	(°C)		($kg\ m^{-3}$)
0.00	-273.15	ORTHO	19254.90
50.00	-223.15	ORTHO	19230.89
150.00	-123.15	ORTHO	19174.69
250.00	-23.15	ORTHO	19107.56
273.00	-0.15	ORTHO	19090.57
295.00	21.85	ORTHO	19073.79
350.00	76.85	ORTHO	19029.50
450.00	176.85	ORTHO	18940.52
550.00	276.85	ORTHO	18840.61
650.00	376.85	ORTHO	18729.77
750.00	476.85	ORTHO	18608.01
850.00	576.85	ORTHO	18475.32
942.02	668.87	ORTHO	18343.57
942.03	668.88	TETRA	18157.33
950.00	676.85	TETRA	18150.62
1048.99	775.84	TETRA	18067.33
1049.00	775.85	BCC	17935.16
1050.00	776.85	BCC	17934.03
1150.00	876.85	BCC	17820.76
1250.00	976.85	BCC	17707.50
1350.00	1076.85	BCC	17594.23
1407.99	1134.84	BCC	17528.55
1408.00	1134.85	LIQUID	17165.22
1450.00	1176.85	LIQUID	17099.81
1550.00	1276.85	LIQUID	16944.06
1650.00	1376.85	LIQUID	16788.31
1750.00	1476.85	LIQUID	16632.57
1850.00	1576.85	LIQUID	16476.82

Table 6: Tabular recommended values for the density of uranium with temperature.

Temperature		Phase	Thermal Conductivity
(K)	(°C)		(W m ⁻¹ K ⁻¹)
0.00	-273.15	ORTHO	NA
50.00	-223.15	ORTHO	33.899
150.00	-123.15	ORTHO	25.021
250.00	-23.15	ORTHO	26.077
273.00	-0.15	ORTHO	26.514
295.00	21.85	ORTHO	26.938
350.00	76.85	ORTHO	28.022
450.00	176.85	ORTHO	30.086
550.00	276.85	ORTHO	32.267
650.00	376.85	ORTHO	34.567
750.00	476.85	ORTHO	36.985
850.00	576.85	ORTHO	39.521
942.02	668.87	ORTHO	41.959
942.03	668.88	TETRA	41.96
950.00	676.85	TETRA	42.176
1048.99	775.84	TETRA	44.919
1049.00	775.85	BCC	44.92
1050.00	776.85	BCC	44.948
1150.00	876.85	BCC	47.839
1250.00	976.85	BCC	50.847
1350.00	1076.85	BCC	53.974
1407.99	1134.84	BCC	55.841
1408.00	1134.85	LIQUID	52.876
1450.00	1176.85	LIQUID	53.668
1550.00	1276.85	LIQUID	55.554
1650.00	1376.85	LIQUID	57.44
1750.00	1476.85	LIQUID	59.326
1850.00	1576.85	LIQUID	61.212

Table 7: Tabular recommended values for the thermal conductivity of uranium with temperature.

Temperature		Phase	Specific Heat
(K)	(°C)		(J kg ⁻¹ K ⁻¹)
0.00	-273.15	ORTHO	0.000
50.00	-223.15	ORTHO	64.939
150.00	-123.15	ORTHO	102.506
250.00	-23.15	ORTHO	112.202
273.00	-0.15	ORTHO	114.123
295.00	21.85	ORTHO	115.937
350.00	76.85	ORTHO	120.477
450.00	176.85	ORTHO	129.224
550.00	276.85	ORTHO	139.233
650.00	376.85	ORTHO	151.121
750.00	476.85	ORTHO	165.454
850.00	576.85	ORTHO	182.783
942.02	668.87	ORTHO	201.844
942.03	668.88	TETRA	180.271
950.00	676.85	TETRA	180.258
1048.99	775.84	TETRA	180.103
1049.00	775.85	BCC	163.609
1050.00	776.85	BCC	163.609
1150.00	876.85	BCC	163.609
1250.00	976.85	BCC	163.609
1350.00	1076.85	BCC	163.609
1407.99	1134.84	BCC	163.609
1408.00	1134.85	LIQUID	200.846
1450.00	1176.85	LIQUID	201.122
1550.00	1276.85	LIQUID	201.533
1650.00	1376.85	LIQUID	201.684
1750.00	1476.85	LIQUID	201.655
1850.00	1576.85	LIQUID	201.502

Table 8: Tabular recommended values for the specific heat capacity of uranium with temperature.

Temperature		Phase	Thermal Diffusivity
(K)	(°C)		($m^2 s^{-1}$)
0.00	-273.15	ORTHO	NA
50.00	-223.15	ORTHO	2.714e-05
150.00	-123.15	ORTHO	1.273e-05
250.00	-23.15	ORTHO	1.216e-05
273.00	-0.15	ORTHO	1.217e-05
295.00	21.85	ORTHO	1.218e-05
350.00	76.85	ORTHO	1.222e-05
450.00	176.85	ORTHO	1.229e-05
550.00	276.85	ORTHO	1.23e-05
650.00	376.85	ORTHO	1.221e-05
750.00	476.85	ORTHO	1.201e-05
850.00	576.85	ORTHO	1.17e-05
942.02	668.87	ORTHO	1.133e-05
942.03	668.88	TETRA	1.282e-05
950.00	676.85	TETRA	1.289e-05
1048.99	775.84	TETRA	1.38e-05
1049.00	775.85	BCC	1.531e-05
1050.00	776.85	BCC	1.532e-05
1150.00	876.85	BCC	1.641e-05
1250.00	976.85	BCC	1.755e-05
1350.00	1076.85	BCC	1.875e-05
1407.99	1134.84	BCC	1.947e-05
1408.00	1134.85	LIQUID	1.534e-05
1450.00	1176.85	LIQUID	1.561e-05
1550.00	1276.85	LIQUID	1.627e-05
1650.00	1376.85	LIQUID	1.696e-05
1750.00	1476.85	LIQUID	1.769e-05
1850.00	1576.85	LIQUID	1.844e-05

Table 9: Tabular recommended values for the thermal diffusivity of uranium with temperature.

Sources, Residuals, and General Comments

In general, Q factors are only given high confidence at temperatures below 1850 K regardless of the source. The practical reason is to limit the impact of wide variations at extreme temperatures during fitting of the region of interest close to the melting point. Some sources may be regarded more highly due to the techniques used, chemical purity, or the consideration of imperfections.

Residual plots given in this section (data as compared to the reported models) will show large deviations for singular or clusters of data points near transitions. These are not necessarily wildly inaccurate single data points, but instead reflective of uncertainties for the transition temperatures combined with uncertainty in temperature during measurements.

The effect of precise isotopics is largely ignored throughout the document. Nearly all of the references assessed here utilize depleted uranium. The term depleted uranium, without any further specification, is used for any U₂₃₅ content less than the naturally occurring content (0.7 wt.% U₂₃₅). The typical range for depleted uranium is 0.2-0.3 wt.% U₂₃₅ with the remainder as U₂₃₈. The detailed isotopic content, by the nature of radioactivity, is time dependent, making any reported average molar weight inherently inaccurate without frequent testing. These caveats aside, the errors introduced by uncertainty in exact isotopic makeup of otherwise high quality samples is small compared to the uncertainty in other measurements.

Density Source Notes

Although Belashchenko, Smirnova, and Ostrovski (2010) gives density based upon MD simulations, the results are highly regarded since they are compared directly to experimental data. In part, the use for the MD experiments gives some validation to the experimental data cited. Since the results of the MD exactly match that of Fokin (2014) and the original has not been found, that reference is only counted once, but the density values are given a Q of 1. Some of the low temperature data refer to the phase as being BCC (and noted as crystalline BCC), so these near ambient points were given a Q value of 0. It was unclear whether these were in reference to a theoretical retained BCC. Shpil'rajn, Fomin, and Kachalov (1988) is used separately as read from this source.

Data from Boivineau et al. (1993) are all high temperature measurements made through isobaric expansion measurements. The high temperatures result in a relatively low fitting weight due to the arguments given previously. The electrical resistivity data from this study

was used to supplement thermal conductivity within the liquid.

As noted by Rohr and Wittenberg (1970), the Grosse, Cahill, and Kirshenbaum (1961) data was compromised during analysis, showing an incorrect offset. While the trend appears to be more accurate, uranium is confirmed to shrink upon solidification so the higher density liquid that they observed must be incorrect. Rohr and Wittenberg (1970) are considered as very high quality data. Both utilize buoyancy-type experiments.

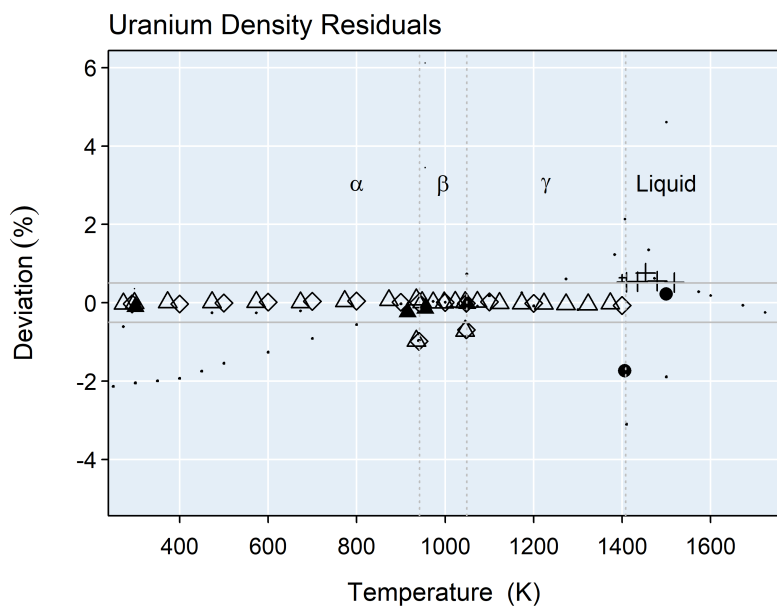
Blank (1998) is different from the other sources because of the theoretical nature of the fractional packing model that is employed rather than physical measurement. That said, the bond lengths were rigorously compared to experimental data, impurity concerns are non-existent, and the model is used to successfully explain diffusion rates within each structure. Due to the nature of the study, no information is obtained for the liquid state.

Yeram Sarkis Touloukian et al. (1975) combines all known measurement sources prior to publication and the recommended values are generally accepted by all investigators barring any more recent measurements. The assessed spline provided by the authors was used with full weight ($Q=1$), but the whole of the underlying data still needs to be included in our records. A critical note is that the original data is in regards to thermal expansion, meaning that a reference state is required in order to convert to density. In this revision the conversion is based upon a density of 19070 kg/m^3 at 293 K . This can be easily changed in the future. Chirkin (1968) is one of the few resources for specific data (rarely if ever cited), but the data appears to be unreliable based upon comparison to all other studies. It appears to be a Russian handbook and so far, we're unable to determine what study the data came from originally. The trends in the data indicate significant systematic error. It is included because we have found values present in other documents that likely originated from this source. See thermal diffusivity measurements for more commentary.

Klepfer and Chiotti (1957) used very high purity uranium in a series of experiments investigating the details of phase transformations with temperature. The density is derived from lattice parameter measurements taken with X-ray diffraction. These measured lattice parameters with temperature are considered among the best early work on the subject.

Beeler et al. (2013) is a computational study of pure uranium that investigates the various allotropic phases. The contribution to this study is the inclusion of the experimental and calculated theoretical density at zero Kelvin. The experimental data trends toward the middle of the selected data.

Bobkov et al. (2008) does not contribute new data, but instead selects particular models for the density (and other properties) of uranium to be used as a nuclear fuel tutorial. Therefore, the selected weighting factor is zero, however, it is included here as a separate listing because of its prominence as an openly available IAEA publication.



Data and weighting updated 22 February, 2021

Figure 5: Source residuals shown as percent deviations relative to the expressions provided in Table 3. The temperature range is limited to the standard metallurgical manufacturing processing range for uranium (295-1700K). Trends in deviation for different datasets are shown. Individual points may show a deviation based on reported temperature as compared to the critical phase transition boundaries used here. Faint gray lines indicate a 1 pct deviation band.

Thermal Conductivity Source Notes

It is critical to note that there is wide discrepancy between data sources at low temperature. This is likely because of both impurity effects and that there are multiple charge density wave transitions in uranium below 43 K which make it nearly impossible to give a single model for uranium at very low temperatures. There is no attempt to resolve this discrepancy here and instead, any user of these recommended values are cautioned relative to low temperatures. Overall, data sources tend to reasonably agree at temperatures between 150 K and the melting point 1408 K. Most of the in-depth studies have been performed for reactor-relevant temperatures (300-850K). The reported properties of the liquid state are troubling in their scarcity and dramatic decrease. Based upon the electrical resistivity data, there is only a modest change in thermal conductivity between BCC and liquid. Due to the very suspect nature of Chirkin (1968) the more modest change is estimated here using the Weidman-Franz law and

the observed changes from Busch, Güntherodt, and Künzi (1970) and Boivineau et al. (1993).

The recommended values from Y. S. Touloukian et al. (1970) should, as usual, be regarded highly since it compiles all work prior to its own publication. Individual curve data points that were recorded in that work are provided, but not given any fitting weight.

Chirkin (1968) is simultaneously an obscure reference, but has seemed to persist in the literature partly due to the temperature range and not necessarily accuracy. The data appears to suffer from systematic errors, especially at high temperature.

Hin (2018) was a recent and major review of thermal conductivity data from 43 K to 940 K. Especially as concerns the orthorhombic phase regime, this document relies heavily upon this review. Takahashi, Yamawaki, and Yamamoto (1988), Howl (1966), Kaity, Pearson, Deem, Babbitt, Hall and Lee (1971), Tyler, and Eriksen are all included in that review, though are not all included in this document's reference library at this time.

Values read from Bobkov et al. (2008) rely upon Krett and Cleveland (1997) and, very oddly, a document that does not contain any metallic uranium data. The report in question is a study on uranium dioxide by Fink and Petri (1997). It is assumed that this is a mistake, but it should be noted that the original reference is unknown.

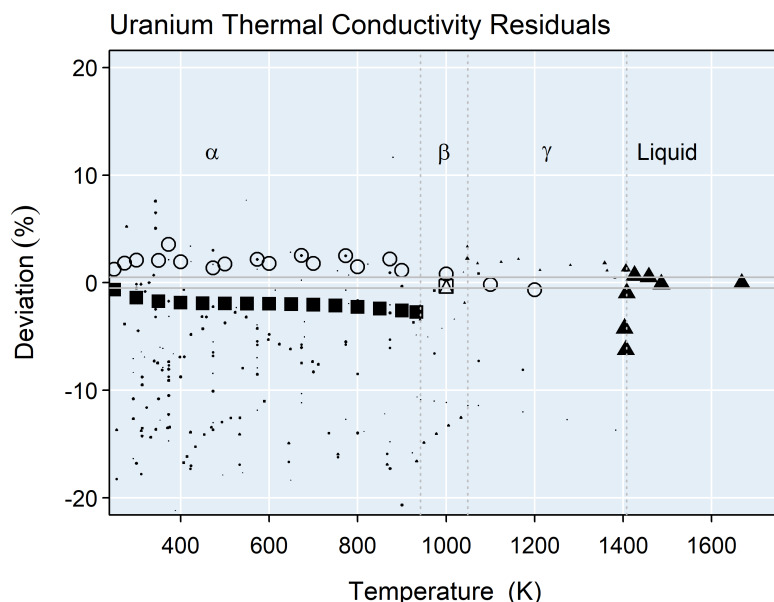


Figure 6: Source residuals shown as percent deviations relative to the expressions provided in Table 4. The temperature range is limited to the standard metallurgical manufacturing processing range for uranium (295-1700K). Trends in deviation for different datasets are shown. Individual points may show a deviation based on reported temperature (therefore phase identification) as compared to the critical phase transition boundaries used here. This is especially true near the melting point. Faint gray lines indicate a 1 pct deviation band.

Specific Heat Capacity Source Notes

Early investigations into the specific heat were performed by Jones, Gordon, and Long (1952), North, and Ginnings. The Jones, Gordon, and Long (1952) data can sometimes be found as (Long, 1942) because the original data was gathered during WWII and only made available in a journal article 10 years later. It should be noted that the data from North (1956) has only been found in database form and not the original document.

Ginnings and Corruccini (1947) provided high temperature data which stood as the best available until the 1970s. It should be highly regarded, however, newer data is likely more accurate. Y. S. Touloukian and Makita (1970) compiled the known data sets for review. Mulford and Sheldon (1988) has extended the range of temperatures. There is a missing data set in the liquid phase that is cited by Mulford and Sheldon (1988) which is currently being obtained.

Marchidan and Ciopec (1976) appears to have systematic errors in both measurements as well as transition temperatures. It is not known how to interpret these differences at this time, so a Q value of 0 has been applied.

Several studies using drop calorimetry have investigated total enthalpy as a function of temperature (Savage and Seibel (1963), Moore and Kelley (1947), and Levinson (1964)). Especially within the narrow temperature bands of beta and gamma (tetrahedral and BCC respectively), the slope is relatively difficult to determine accurately. This is especially true in the beta phase. It is somewhat clear that the data will likely only support a constant heat capacity, though some authors have chosen to fit to a temperature-varying function. The most contradiction, and therefore the highest uncertainty, is in the beta phase data and in the liquid phase simply due to temperature and phase difficulties. The data pulled from these studies is dependent upon differences in enthalpy and on accuracy of temperature data.

The currently selected data are highly consistent with Dinsdale (1991), which does not give direct heat capacity data, but does show thermodynamic consistency between all phase transitions.

Thermal Diffusivity Source Notes

In general the data for thermal diffusivity is quite scattered and has very significant uncertainty at higher temperatures (above 942 K). While diffusivity is often measured independently through a pulse technique, the overall accuracy also suffers from the combined uncertainty of density, thermal conductivity, and specific heat. This makes selection between divergent trends difficult. It should be noted again that none of the thermal diffusivity data presented here is used

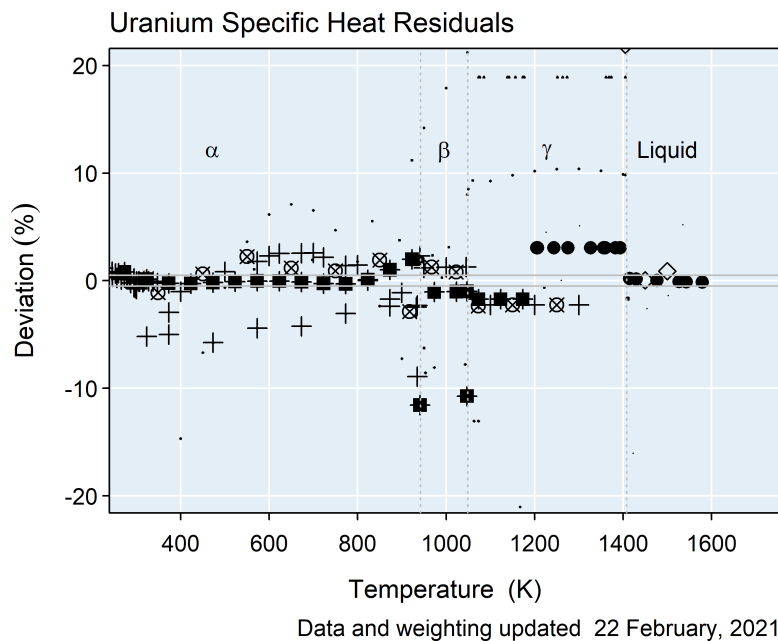


Figure 7: Source residuals for specific heat capacity shown as percent deviations relative to the expressions provided in Table 5. The temperature range is limited to the standard metallurgical manufacturing processing range for uranium (295-1700K). Faint gray lines indicate a 1 pct deviation band.

for fitting of the recommended values and instead is used as a check of the solution by correlation.

Yeram Sarkis Touloukian et al. (1974) is the only rigorous review of thermal diffusivity data for uranium and the temperature range is limited. Therefore, the fact that the current model fits this data quite well, is likely the best that can be currently expected. Chiotti and Carlson (1956) and Nasu et al. (1968) were included in the dataset which resulted in the recommended values, so they are given here only as Q=0 reference points.

Bobkov et al. (2008) gives no reference for the liquid value. This value can possibly be attributed to Chirkin (1968). If this is the correct source, then it would appear that, like that of Chiotti, the higher temperature data seemed to follow a trend that is likely incorrect. Alternatively it may come from data that could not be found at this time. The density for liquid uranium is attributed to Shpil'rajn, Fomin, and Kachalov (1988). Regardless, the data point was included though the lack of attribution make it suspect. Since currently the diffusivity is not used for fitting, the predicted value is considerably higher. For the solid phase, Bobkov et al. (2008) references Krett and Cleveland (1997) and a table of calculated values (by correlation) are based upon the specific heat, density, and thermal conductivity of the fitted forms provided. Krett and Cleveland (1997) provides only a reference to Yeram Sarkis Touloukian et al. (1974) as is done here. In

a future revision of this document, it would be worthwhile to explore the fitted model differences given here and those given in by Bobkov.

Chiotti and Carlson (1956) measured thermal diffusivity in order to gain information on the thermal conductivity. ARMCO iron was used as a reference standard. Multiple annealing treatments were performed and showed considerable variation in the measured diffusivity. The data follow a nearly linear trend with significant deviations at the phase transition boundaries.

Nasu et al. (1968) used the laser pulse technique (Parker analysis) to perform measurements between 293 and 1123 K. Points were read from the graph as individual data were not provided. These show a relatively flat trend with discontinuities at the phase transitions.

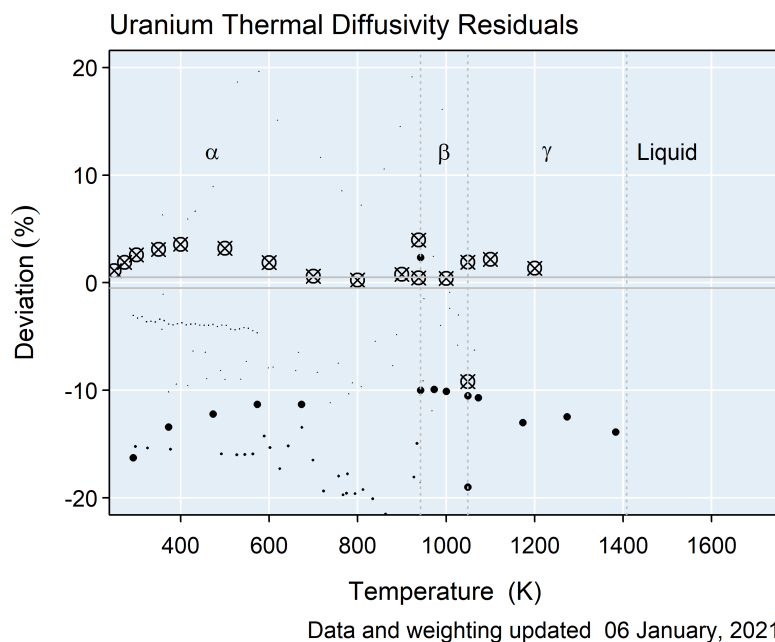


Figure 8: Source residuals for thermal diffusivity are shown as percent deviations relative to the modeled output. The temperature range is limited to the standard metallurgical manufacturing processing range for uranium (295-1700K). Faint gray lines indicate a 1 pct deviation band.

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References

- Allaire, JJ, Yihui Xie, Jonathan McPherson, Javier Luraschi, Kevin Ushey, Aron Atkins, Hadley Wickham, Joe Cheng, and Winston Chang. 2018. *Rmarkdown: Dynamic Documents for r*. <https://CRAN.R-project.org/package=rmarkdown>.
- Beeler, Benjamin, Chaitanya Deo, Michael Baskes, and Maria Okuniewski. 2013. "First Principles Calculations of the Structure and Elastic Constants of Alpha, Beta and Gamma Uranium." Journal Article. *Journal of Nuclear Materials* 433 (1-3): 143–51. doi:10.1016/j.jnucmat.2012.09.019.
- Belashchenko, D. K., D. E. Smirnova, and O. I. Ostrovski. 2010. "Molecular-Dynamic Simulation of the Thermophysical Properties of Liquid Uranium." Journal Article. *High Temperature* 48 (3): 363–75. doi:10.1134/S0018151X10030107.
- Blank, H. 1998. "Fractional Packing Densities and Fast Diffusion in Uranium and Other Light Actinides." Journal Article. *Journal of Alloys and Compounds* 268 (1-2): 180–87. doi:10.1016/S0925-8388(97)00604-X.
- Bobkov, V, L Fokin, E Petrov, V Popov, V Rumiantsev, and A Savatimsky. 2008. "Thermophysical Properties of Materials for Nuclear Engineering: A Tutorial and Collection of Data." Report.

- Boivineau, M., L. Arlès, J. M. Vermeulen, and Th Thévenin. 1993. "High-Pressure Thermophysical Properties of Solid and Liquid Uranium." Journal Article. *Physica B: Condensed Matter* 190 (1): 31–39. doi:10.1016/0921-4526(93)90439-D.
- Busch, G., H. J. Güntherodt, and H. U. Künzi. 1970. "Hall Coefficient and Electrical Resistivity of Liquid Uranium." Journal Article. *Physics Letters A* 32 (6): 376–77. doi:10.1016/0375-9601(70)90007-1.
- Chiotti, P., and O. N. Carlson. 1956. "HANFORD SLUG PROGRAM SEMI-ANNUAL SUMMARY RESEARCH REPORT FOR JULY 1 TO DECEMBER 31 1955." Report. doi:10.2172/4375107.
- Chirkin, V S. 1968. *Thermophysical Properties of Materials for Nuclear Technology*. Book.
- Dinsdale, A T. 1991. "SGTE Data for Pure Elements." Journal Article. *Calphad* 15 (4): 317–425. doi:10.1016/0364-5916(91)90030-N.
- Erez, Gidon, and Uzy Even. 1966. "The Wiedemann—Franz Ratio of Metallic Uranium at Elevated Temperatures." Journal Article. *Journal of Applied Physics* 37 (13): 4633–34. doi:10.1063/1.1708108.
- Fokin, L. R. 2014. *Liquid Uranium Density Isobar, Melting Line, Critical Temperature Assessment*. Book. Zhidkij Uran: Izobara Plotnosti, Liniya Plavleniya, Otsenka Kriticheskoy Temperatury. Russian Federation: FGUP GNTs RF - FEHL. http://inis.iaea.org/search/search.aspx?orig_q=RN:46094355.
- Ginnings, Defoe C, and RJ Corruccini. 1947. "Heat Capacities at High Temperatures of Uranium, Uranium Trichloride, and Uranium Tetrachloride." Journal Article. *Journal of Research of the National Bureau of Standards* 39: 309–16.
- Grosse, A. V., J. A. Cahill, and A. D. Kirshenbaum. 1961. "Density of Liquid Uranium." Journal Article. *Journal of the American Chemical Society*, 4665–66.
- Hall, R. O. A., and J. A. Lee. 1971. "The Thermal Conductivity of Alpha Uranium Between 5 and 100 k." Journal Article. *Journal of Low Temperature Physics* 4 (4): 415–19. doi:10.1007/BF00628741.
- Hin, Celine. 2018. "Thermal Conductivity of Metallic Uranium." Report. Virginia Polytechnic Institute; State University (Virginia Tech). doi:10.2172/1433931.
- Howl, D. A. 1966. "The Thermal Conductivity of Springfields Adjusted Uranium in the Temperature Range 160–620° c." Journal Article. *Journal of Nuclear Materials* 19 (1): 9–14. doi:10.1016/0022-3115(66)90124-3.

- Jones, W M, Joseph Gordon, and E A Long. 1952. "The Heat Capacities of Uranium, Uranium Trioxide, and Uranium Dioxide from 15°k to 300°k." Journal Article. *The Journal of Chemical Physics* 20 (4): 695–99. doi:10.1063/1.1700518.
- Klepfer, Harold H, and P Chiotti. 1957. "Characteristics of the Solid State Transformations in Uranium." Thesis. https://lib.dr.iastate.edu/ameslab_iscreports/163.
- Krett, V, and J Cleveland. 1997. *Thermophysical Properties of Materials for Water Cooled Reactors*. Book. Vol. 949. TECDOC Series. Vienna: International Atomic Energy Agency. <https://www.iaea.org/publications/5601/thermophysical-properties-of-materials-for-water-cooled-reactors>.
- Levinson, L. S. 1964. "Heat Content of Molten Uranium." Journal Article. *The Journal of Chemical Physics* 40 (12): 3584–85. doi:10.1063/1.1725055.
- Marchidan, D. I., and M. Ciopec. 1976. "Enthalpy of Uranium to 1500 k by Drop Calorimetry." Journal Article. *The Journal of Chemical Thermodynamics* 8 (7): 691–701. doi:10.1016/0021-9614(76)90021-5.
- Moore, G. E., and K. K. Kelley. 1947. "High-Temperature Heat Contents of Uranium, Uranium Dioxide and Uranium Trioxide1." Journal Article. *Journal of the American Chemical Society* 69 (9): 2105–7. doi:10.1021/ja01201a009.
- Mulford, R. N. R., and R. I. Sheldon. 1988. "Density and Heat Capacity of Liquid Uranium at High Temperatures." Journal Article. *Journal of Nuclear Materials* 154 (2-3): 268–75. doi:10.1016/0022-3115(88)90363-7.
- Nasu, Shoichi, Susumu Fukushima, Toshihiko Ohmichi, and Takeo Kikuchi. 1968. "Thermal Diffusivity of Uranium by Laser Pulse Method from 20°to 850°c." Journal Article. *Japanese Journal of Applied Physics* 7: 682–82.
- R Core Team. 2018. *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing. <https://www.R-project.org/>.
- . 2020. *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing. <https://www.R-project.org/>.
- Rohr, W G, and L J Wittenberg. 1970. "Density of Liquid Uranium." Journal Article. *Journal of Physical Chemistry* 74 (5): 1151–52. doi:10.1021/j100700a035.
- Savage, H., and R. D. Seibel. 1963. "Heat Capacity Studies of Uranium and Uranium-Fissium Alloys." Report ANL-6702.

- Argonne National Laboratory. <https://digital.library.unt.edu/ark:/67531/metadc866865/>.
- Shpil'rajn, Eh Eh, V. A. Fomin, and V. V. Kachalov. 1988. "Density and Surface Tension of Uranium in Liquid Phase." Journal Article. *Teplofizika Vysokikh Temperatur* 26 (5): 892–900. http://inis.iaea.org/search/search.aspx?orig_q=RN:20040718.
- Takahashi, Yoichi, Michio Yamawaki, and Kazutaka J Yamamoto. 1988. "Thermophysical Properties of Uranium-Zirconium Alloys." Journal Article. *Journal of Nuclear Materials* 154 (1): 141–44.
- Touloukian, Y S, and T Makita. 1970. "Thermophysical Properties of Matter - the TPRC Data Series. Volume 6. Specific Heat - Nonmetallic Liquids and Gases. (Reannouncement). Data Book." Report AD-A-951940/6/XAB; Other: CNN: F33615-68-C-1229 United States Other: CNN: F33615-68-C-1229 NTIS GRA English. ; Purdue Univ., Lafayette, IN (United States). Thermophysical; Electronic Properties Information Center.
- Touloukian, Y S, R W Powell, C Y Ho, and P G Klemens. 1970. "Thermophysical Properties of Matter - the TPRC Data Series. Volume 1. Thermal Conductivity - Metallic Elements and Alloys. (Reannouncement). Data Book." Report AD-A-951935/6/XAB; Other: CNN: F33615-68-C-1229 United States Other: CNN: F33615-68-C-1229 NTIS GRA English. ; Purdue Univ., Lafayette, IN (United States). Thermophysical; Electronic Properties Information Center.
- Touloukian, Yeram Sarkis, RK Kirby, RE Taylor, and PD Desai. 1975. "Thermophysical Properties of Matter-the Tprc Data Series. Volume 12. Thermal Expansion Metallic Elements and Alloys." Report. THERMOPHYSICAL AND ELECTRONIC PROPERTIES INFORMATION ANALYSIS CENTER . . .
- Touloukian, Yeram Sarkis, RW Powell, CY Ho, and MC Nicolaou. 1974. "Thermophysical Properties of Matter-the TPRC Data Series. Volume 10. Thermal Diffusivity." Report. Thermophysical; Electronic Properties Information Analysis Center . . .
- Turchi, Patrice E. A. 2018. "Thermodynamic, Kinetic, and Physical Properties of Nb-u (Niobium-Uranium)." Report LLNL-TR-752281; Other: 937482 United States 10.2172/1459121 Other: 937482 External Audience (Unlimited) LLNL English. ;Lawrence Livermore National Lab. (LLNL), Livermore, CA (United States). <https://www.osti.gov/servlets/purl/1459121>.